

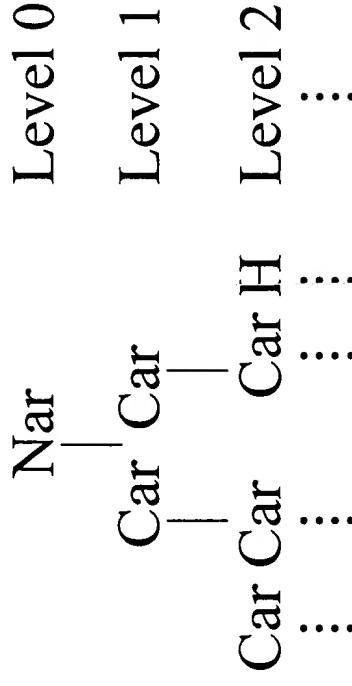
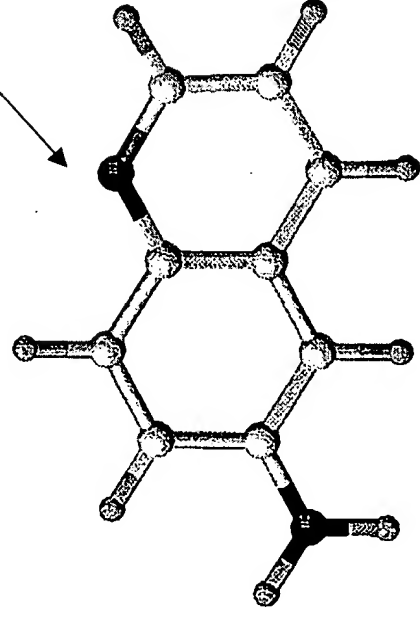
FIGURE 1

Environment Around an Ionizable Center

- E.g. 6-aminoquinoline

Start with interesting atom find connections

Measured 5.6
predicted 5.0



String contains a bin for each required atom type at each level, the number of atom types is accumulated to form the string

FIGURE 3

Environment Around an Ionizable Center

- In addition to atom types, certain group types are also used and improve the performance of the algorithm

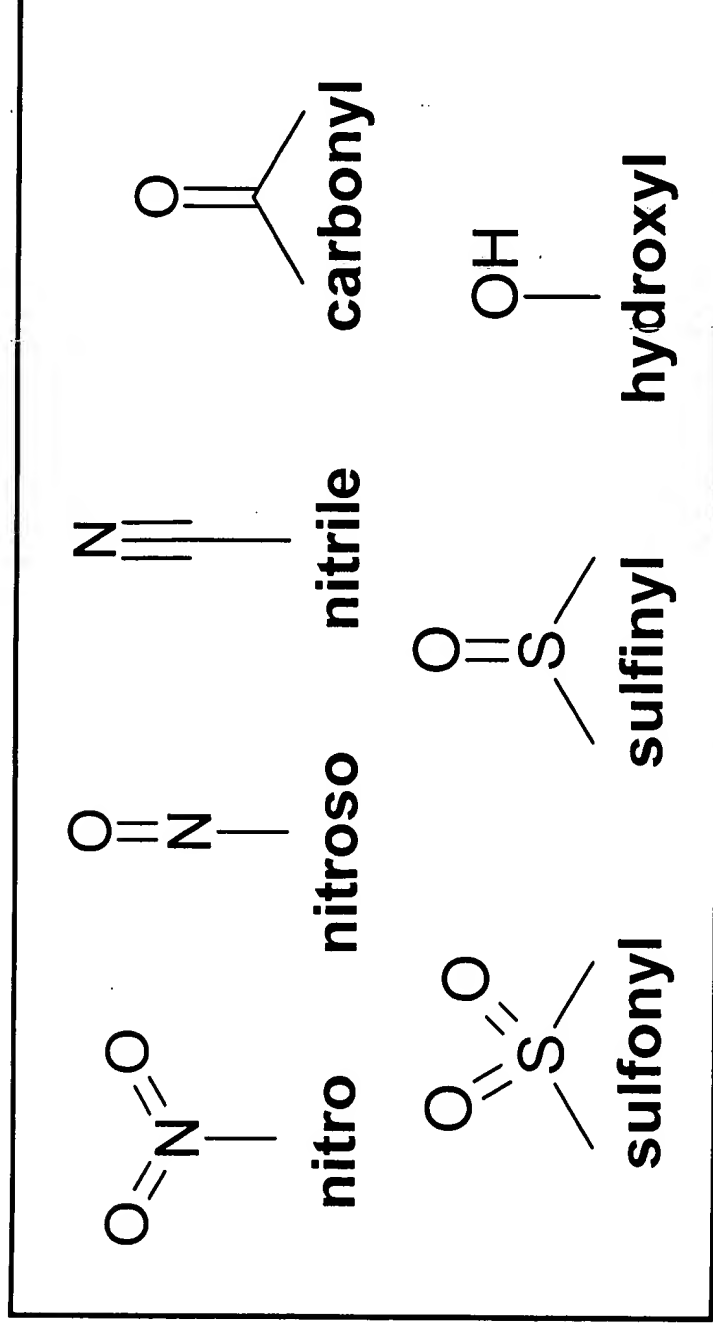
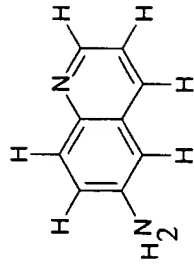


FIGURE 4



Atom Type:	C.3	C.2	C.1	C.ar	C.cat	N.3	N.2	N.1	N.ar	N.am	N.pl3	N.4	O.3	O.2	O.CO2	S.3	S.2	S.O	S.O2	P.3	H	F	CL	BR	I	NO2	NO	CN	CO	SO2	SO	OH
Level 0								1																								
Level 1				2																												
Level 2				3																1												
Level 3				3																2												
Level 4				1																3												
Level 5											1																					



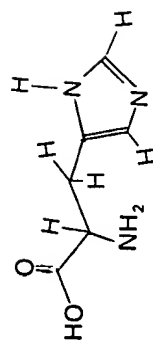


FIGURE 5

[illegible]



Construction of the hierarchical tree from one example, 6-amino quinoline

FIGURE 7

pK_a of Bases (384)

PC = 5, $r^2=0.922$ $q^2=0.832$, Std. Err = 0.89

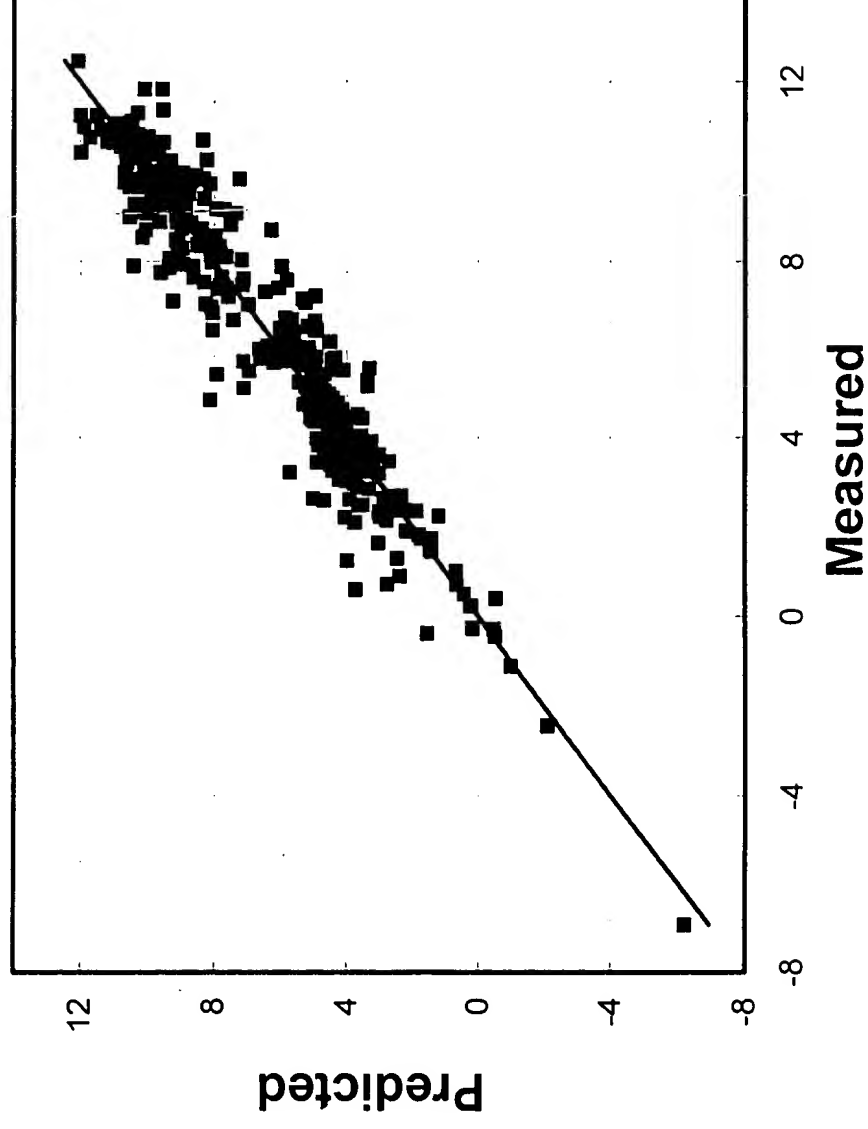


FIGURE 8

pK_a of Acids (646)

PC = 6, $r^2 = 0.927$, $q^2 = 0.792$, Std. Err = 0.77

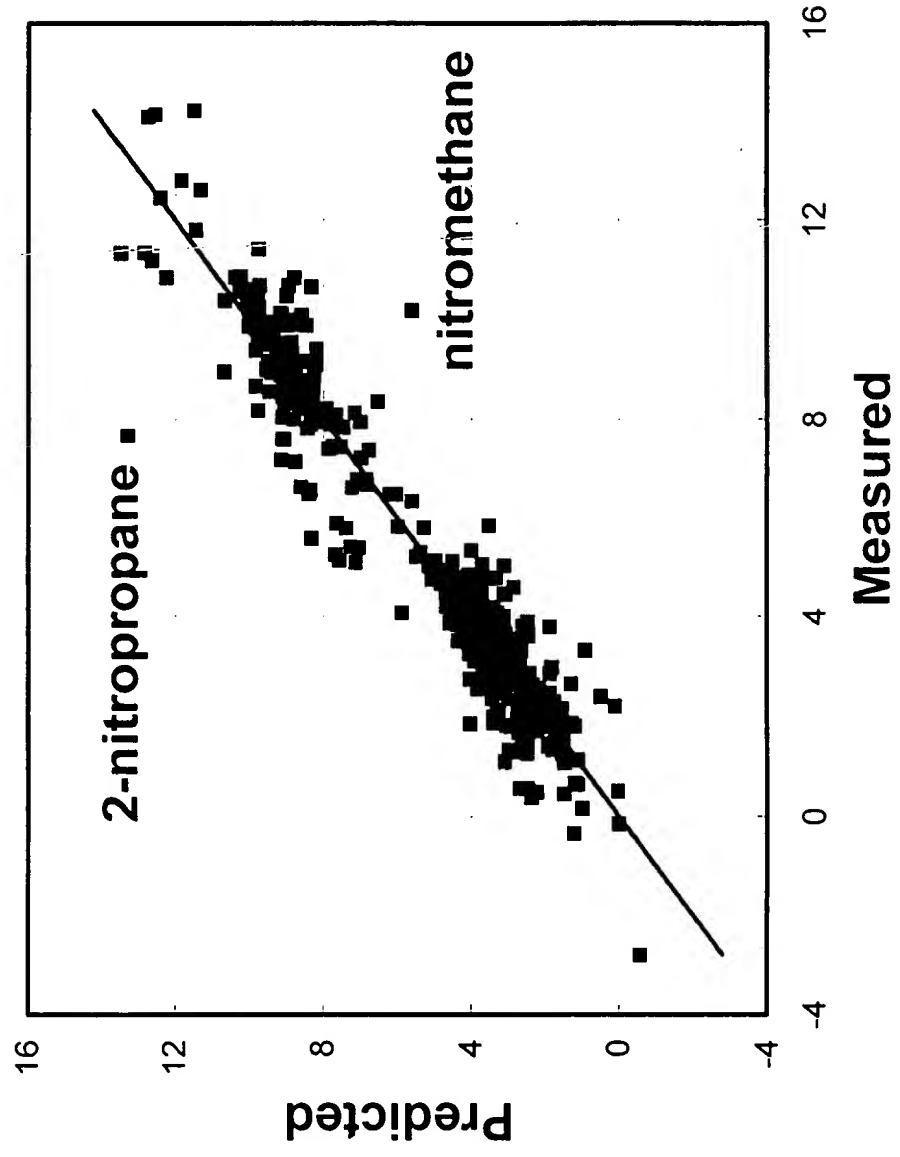
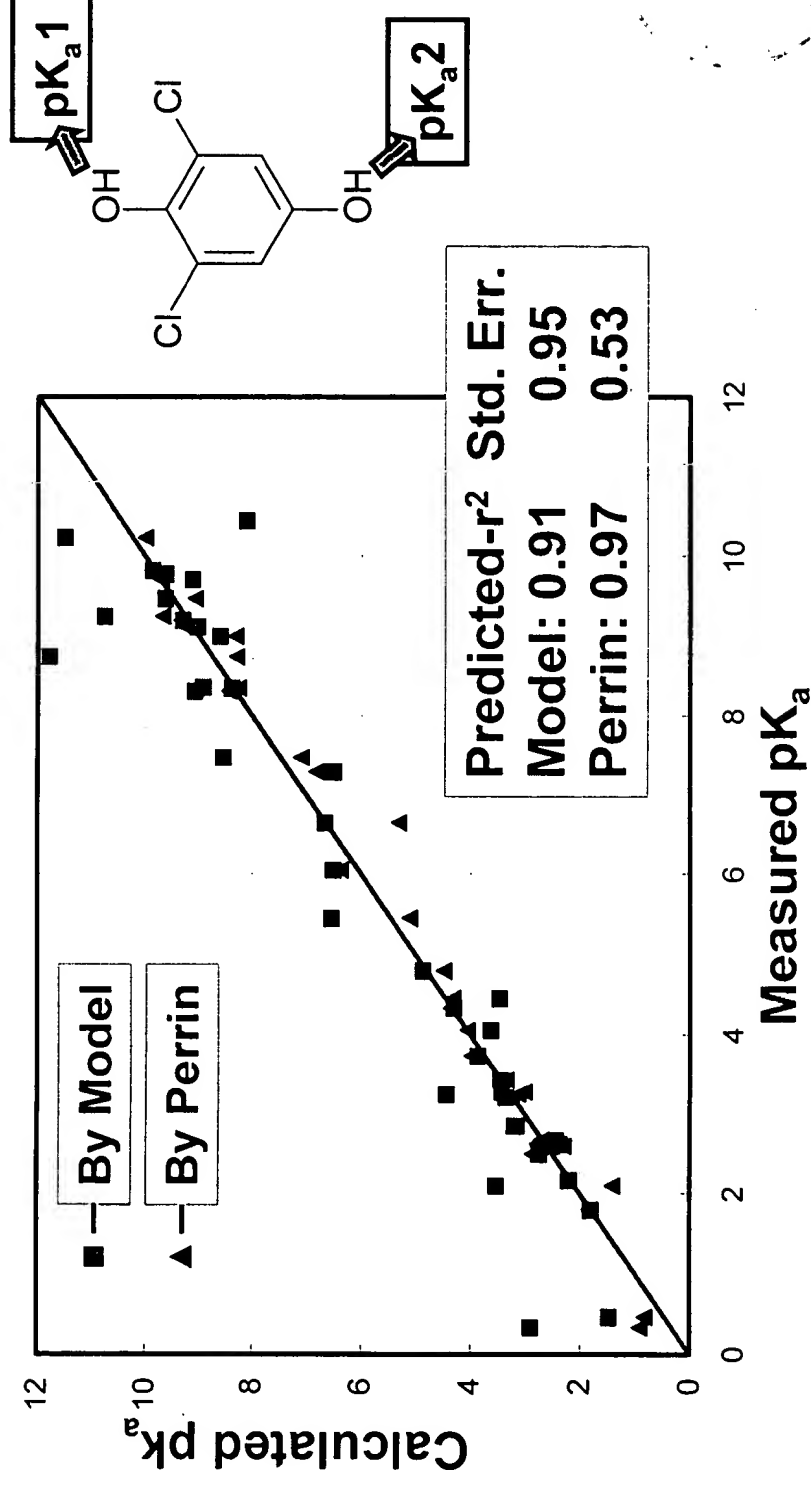


FIGURE 9

Prediction on Molecules

- 37 acid and base molecules selected by Perrin* *et al.* as examples, and were not included in the training set
- For molecules containing multiple ionizable centers the model correctly predicted the order for all of them, ie



*Perrin DD, Dempsey B, Serjeant EP, *pKa prediction for organic acids and bases*, Chapman and Hall, London, 1981.